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Modeling to Build a Better Fuel Cell

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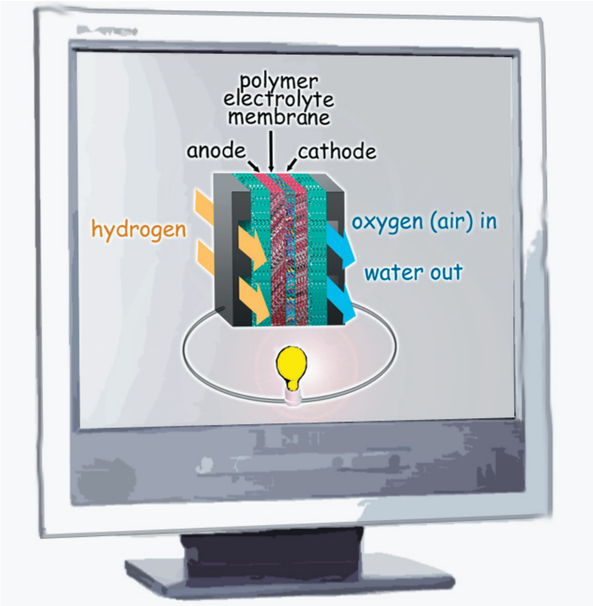

On the one hand, fuel cells are touted as a clean, sustainable energy solution; on the other, they are dismissed as too expensive and too far from market. Behind the contradictory perceptions lies a technology suitable for many applications—and rich in variations. Among the problems that need solving before fuel cells become common in the marketplace are lowering their cost and increasing the durability of their materials—and developing clean, sustainable ways to generate, distribute, and store hydrogen, the fuel cell's fuel.

Computer modeling is one of the tools scientists are using to bring fuel cells closer to technical and economic viability.

"Fuel cells are costly to study in the laboratory," says Adam Weber of Berkeley Lab's Environmental Energy Technologies Division (EETD), who uses computer models to simulate what goes on inside fuel cells. "It's very hard to characterize what's going on in a fuel cell locally. Imaging techniques are difficult and expensive to use in a cell's interior, and the resolution of existing techniques is often not high enough."

Computer simulation of the processes in the cell, however, is a cost-effective way to figure out what's going on inside. "It let's you think outside the box," Weber says. "What if we made a new electrode material? What properties should it have? Simulation provides an approximate idea of the distribution of heat, fuel, and water within different parts of the cell, and how these distributions affect the cell's power output."

One of Weber's projects is studying thermal and water management in polymer-electrolyte fuel cells (PEFCs) using computer simulation. Understanding the flow of water in a fuel cell is important, because if water is not managed properly the fuel cell will not produce its maximum power, let alone operate. In the long term, improper water management could also lead to shorter fuel-cell lifetime, which affects the economic viability of the technology. The ultimate goal of the research is to provide guidance to other scientists and fuel cell manufacturers so that they can optimize fuel cell performance at minimum cost.

Where does the water come from?

"The fuel cell is an energy conversion device, not an energy storage device like a battery," Weber explains. The conversion process begins with hydrogen, the fuel input. Hydrogen flows into the fuel cell and encounters a gas diffusion layer, where it spreads out evenly on a plane.

The gas now reacts with electrolyte at the cell's anode layer, resulting in the dissociation of hydrogen into protons and electrons. The electrons are the cell's power output—they flow out of the cell as an electric current and do useful work, such as moving an automobile or providing electricity to a building or space vehicle.

The rest of the hydrogen gas, the positively charged protons, flows through the electrolyte, a negatively charged polymer termed an ionomer, to the cathode layer. The electrolyte is crucial: its role is to conduct protons, not electrons or gas.

At the cathode, in a series of chemical reactions, the protons recombine with electrons and with oxygen, which is flowing into the cell from the atmosphere, to form water—the primary source of the water within the cell.

The material that forms a fuel cell's electrolyte defines the type of fuel cell. Weber's research focuses on polymer-electrolyte fuel cells, considered promising for automotive and small, stationary applications, with operating temperatures usually less than 100°C (212°F). The typical material in use today consists of fluorinated polymers (Teflon, for example) with acid-group side chains.

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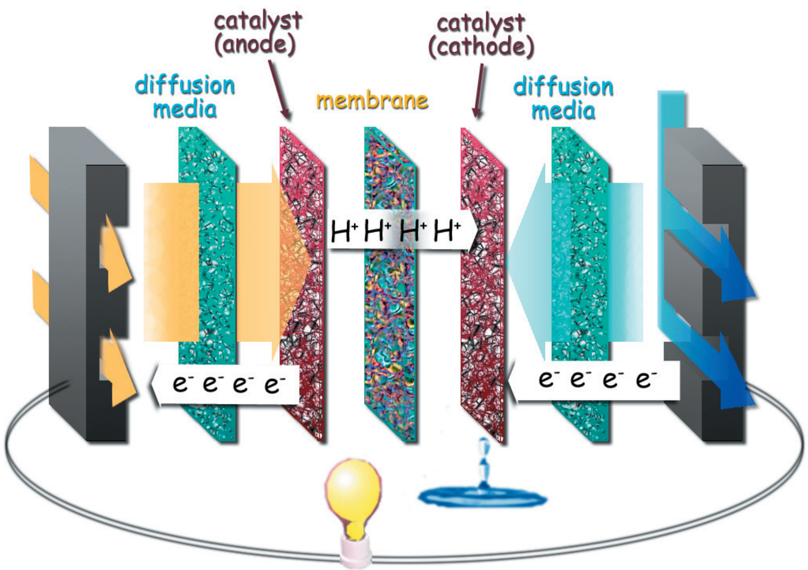


How a fuel cell works: hydrogen (yellow) fed into the cell diffuses to the anode catalyst and reacts to form protons and electrons. The protons migrate through the membrane, while the electrons form a current in an external circuit. Meanwhile, oxygen (blue) from air diffuses to the cathode catalyst layer, where it reacts with protons that have crossed the barrier and electrons arriving from the circuit, to form water.

In solid-oxide fuel cells, the electrolyte is a ceramic that conducts oxygen ions. Solid-oxide fuel cells operate at much higher temperatures, more than 700°C (1,260°F). Solid-oxide fuel cells are considered ideal for stationary applications, such as powering buildings, thanks to their cogeneration capabilities and use of natural gas as a fuel.

Dueling Trends

A fuel cell that is generating an electrical current is also generating heat and water. The water in the cell is either liquid or a vapor, depending on the local temperature at the point in the cell where the water is passing through.

The polymer electrolyte needs to be wet in order to conduct efficiently, so some liquid water in the ionomer separating the anode from the cathode is desired. Liquid water also hydrates the membrane much better than water vapor. However, if liquid water fills up the pore pathways in the diffusion layer and blocks access of the reactant gases to the reaction sites, more vapor and less liquid is desirable.

"This is an optimization problem," says Weber. "The problem is to keep sufficient water in the membrane so it can do its job of conducting, without having too much in the cell. The structure of an optimized backing layer depends on factors like the number and size of pores in the layer, their distribution, and total porosity."

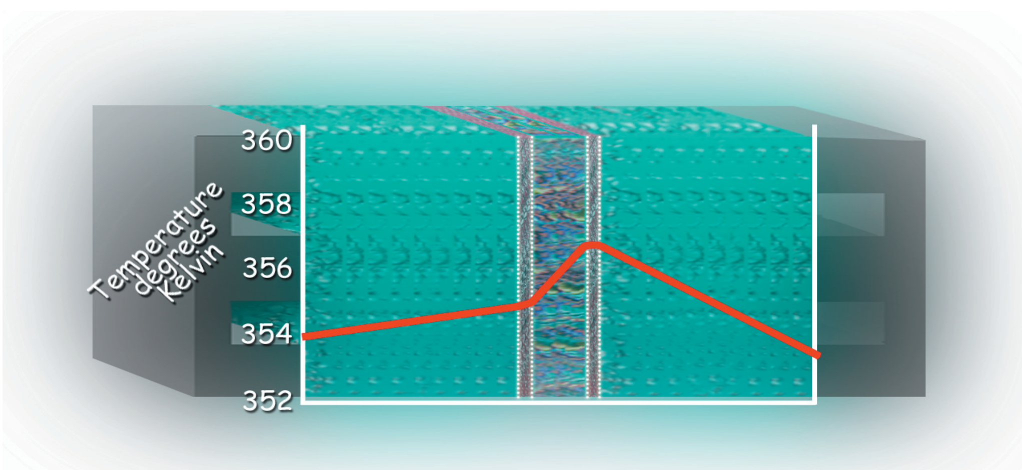
Weber's computer simulations show that the shape of the gradient, the temperature profile of the fuel cell, reflects the cell's water distribution and management, with trade-offs for performance. Temperature reaches a maximum at the cathode where the oxygen is reduced to water—an inefficient reaction. Water vapor moves out of the cell in the diffusion layers; meanwhile the temperature decreases from the cathode to the gas channels.

Higher temperatures increase the rate of chemical reactions, the diffusion of reactant gases, and the conductivity of the electrolyte—all to the good, because these factors tend to increase power output. But higher temperatures at the membrane dilute liquid water; water vapor dilutes the reactants in the cell; and the flow of water vapor out of the cell inhibits hydrogen and oxygen from entering.

Weber's simulation results suggest that these latter effects are the dominating factors, reducing the cell's performance if the vapor is not managed. The simulations show water vapor moving out of the cell and condensing, while liquid water moves into the cell—all because of the temperature gradient.

"A lot of water is moving through the cell because of condensation of the vapor to liquid, and evaporation of the liquid to vapor," says Weber. "Water is also changing from liquid to vapor and back at the membrane. But these heat-related effects almost exactly balance each other in the cell."

Simple measurements of the inputs and outputs of the cell would not explain what is going on inside it. "In fact," says Weber, "only a degree or so temperature gradient at 80°C can move as much water as the cell generates—and results in more absolute heat effects than that generated by the electrochemical reactions."



Temperature reaches a maximum at the cathode, where oxgen is reduced to water. Temperature distribution inside the fuel cell has significant effects on performance.

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A design for better water and thermal management

Weber points out that there are several engineering solutions to the water and thermal management problem. “You can tailor a microporous layer to do a better job of keeping liquid water in contact with the membrane. Wicks or porous plates can help remove excess liquid water. Distributed liquid-water injections can help maximize the liquid water at the membrane and reduce the temperature, so that less water vapor forms. You can induce temperature gradients to move water where you want it.”

Because of Weber’s work, enough is now known about the temperature and moisture conditions inside polymer-electrolyte fuel cells to point fuel cell designers in the right direction to solve these problems. But other, large challenges remain.

“The materials problem is the big one,” says Weber. “We need a better membrane material for higher temperature conditions in the fuel cell.” Operating the cell at higher temperatures, above 100°C, increases efficiency and power output but degrades the cell faster, shortening its lifetime.

Weber and EETD researcher John Kerr are conducting research in this area to model and create membrane materials capable of operating at elevated temperatures. Weber is also working on computer models that relate the impacts of material tolerances and manufacturing defects, a key route for eventual large-scale fuel cell production. Their goal is to help develop the materials that can meet goals established by the Department of Energy’s fuel-cell research program.

Among these goals are fuel cells that will last 5,000 hours (equivalent to about 150,000 miles of driving), cost less than $50 per kilowatt—automobile combustion engines currently cost $30 to $35 per kilowatt—and operate at the full range of environmental conditions as cars powered by internal combustion engines, from extreme cold in winter to hot, humid summer conditions. The fuel cells will also have to start up quickly and reach 50 percent of rated power within 30 seconds—combustion engines turn on very quickly, but current fuel cells have a slower start-up curve.

There’s still plenty to do!

Additional information

More about the Department of Energy’s fuel-cell research is at http://hydrogen.energy.gov/fuel_cells.html.

For more on Berkeley Lab research on novel polymer materials, visit http://www.lbl.gov/Science-Articles/Archive/sabl/2007/Nov/polymer.html.

More on Berkeley Lab research on catalysis in polymer-electrolyte membranes can be found at http://www.lbl.gov/Science-Articles/Archive/MSD-H-fuel-cells.html.

More on Berkeley Lab research on solid-oxide fuel cells is at http://www.lbl.gov/Science-Articles/Archive/MSD-fuel-cells.html.

For more on Berkeley Lab research on hydrogen storage, visit http://www.lbl.gov/Science-Articles/Archive/sabl/2005/August/01-hydrogen-future.html.